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BFIT—A Program to Analyze and Fit the BCJ Model Parameters to Experimental Data

Tutorial and User's Guide

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Abstract

While the BCJ plasticity model is very powerful in representing material behavior, finding values for the twenty parameters representing a particular material can be a daunting task. Bfit was designed to make this task at least feasible if not easy. The program has been developed over several years and incorporates the suggestions and requests of several users.

Introduction

The temperature and rate dependent plasticity model developed by D. Bammann, M. Chiesa and G. Johnson[1,2], and the damage model developed by Bammann and M. Chiesa [3,4] require twenty parameters relating hardening and recovery to temperature and strain rate. These models are available in the Sandia mechanical codes PRONTO2D, PRONTO3D, JAC2D, JAC3D, and JAS3D as well as ABAQUS and DYNA3D. This program is designed to help in the understanding of those parameters and to select parameter values appropriate to a user's problem.

The damage model requires another parameter to describe damage or void growth. Determination of that parameter requires matching notched bar experiments using a mechanical finite element code and is beyond the scope of this program.

To run bfit, you need to log into a UNIX computer. If you are using the Sandia compute servers FRANKLIN or SAHP046 from an X terminal you will need to set the environmental variables DISPLAY and XENVIRONMENT. If you are using the C shell, this is done with the commands

```
setenv DISPLAY xxxx:0.0
setenv XENVIRONMENT ~lathrop/newfit/Bfit
```

From the Bourne shell use

```
DISPLAY=xxxx:0.0
XENVIRONMENT=~lathrop/newfit/Bfit
export DISPLAY
export XENVIRONMENT
```

Where xxxx is the network name of your terminal.

Then run `~lathrop/newfit/bfit`

On other systems, you will need to find the directory that contains bfit and Bfit.

You can avoid setting XENVIRONMENT by storing a copy of the resource file Bfit in your home directory. This might be the easiest way to work. **Don't run bfit** without this file, since it creates many of the button labels and messages used in bfit.

Understanding the Model

The Parameters

The BCJ model requires up to twenty parameters to describe the temperature and strain rate dependent behavior of a material. However, there are only 9 terms, but they are temperature dependent and require at least two parameters to determine their value. For most of the terms, that value is determined by an equation of the form

$$parameter = c1 \bullet \exp\left(\frac{-c2}{temp}\right).$$

The actual temperature dependence for each term is shown in table 1.

The nine terms can be logically grouped into threes. The first three are *V, Y* and *f* which specify the yield stress, with *Y* specifying the rate independent part and *V* and *f* the rate dependence. The second three *rd, h* and *rs* describe the tensor or kinematic hardening and recovery, which can be thought of as the center of the yield surface. Finally, *Rd, H* and *Rs* describe the scalar or isotropic hardening and recovery, which can be thought of as the radius of the yield surface.

Using the code to examine the model

Let's start up the program and look at the model. Begin the code by following the directions on page 2.

You should see something that looks like figure 1.

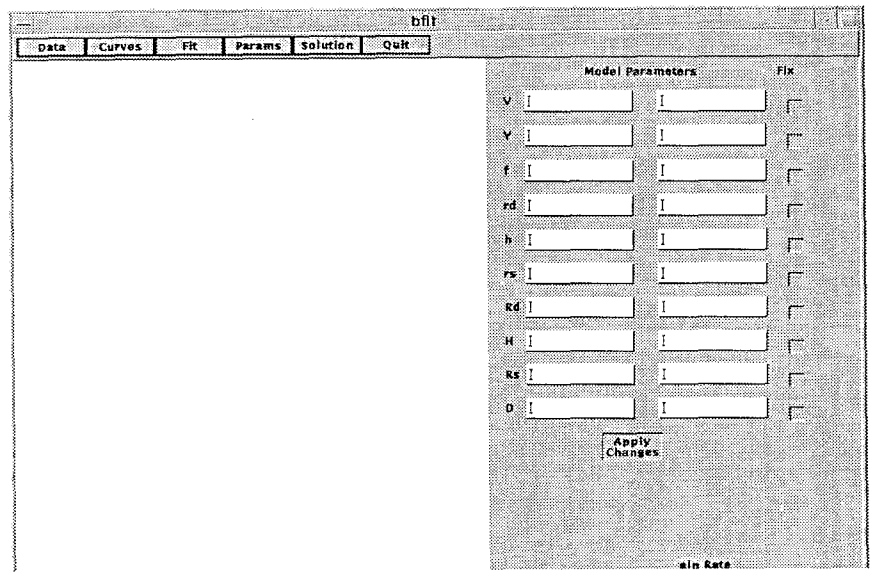


FIGURE 1. Beginning of bfit program

Since each parameter has a constant value and a temperature dependent part, they are displayed by those pairs. Since $V = C_1 \exp\left(\frac{-C_2}{Temp}\right)$, both C_1 and C_2 are displayed next

to V. Similarly C_3 and C_4 are shown next to Y. So the odd term or constant term is in the first column.

Model Parameters

Setting Elastic Moduli

To begin, we will need to describe the elastic part of the material, so pick PARAMS in the menu bar and slide down and select Set Young's Modulus & Poisson's Ratio from the menu. This will bring up an empty table in which you can enter temperature dependent values for Young's Modulus and Poisson's Ratio. As an example, enter a temperature of 100, 1.0e5 for Young's modulus, and 0.3 for Poisson's ratio. Then click on the OK button. Since we entered only one temperature, the program knows to use these values for Young's Modulus and Poisson's Ratio at all temperatures. You can specify temperature dependent values by entering values at more than one temperature, but be sure the temperatures cover the temperatures you will be using or else an error message will appear when you try to use a temperature outside that range. *The program will not extrapolate!* We could have entered values for the bulk and shear moduli instead of Young's modulus and Poisson's ratio. You can check this by selecting Set Bulk and

Shear from the menu (under PARAMS) and see that we now have values for these. They were calculated from the values you just entered.

Developing a Model

Elastic - Perfectly Plastic

We will begin with a simple elastic-perfectly plastic model. In the area for Model Parameters enter 135 next to Y (this will give an elastic perfectly plastic material with a yield stress of 135). To make sure the program got this value, click on the Apply Changes button. Now, pick Curves from the menu bar and select Add curves under uniaxial. A form will appear asking for temperature and strain rate. Since we haven't introduced any temperature or rate dependence yet, almost any values will work here, but for now enter 300 for temperature and .01 for strain rate.

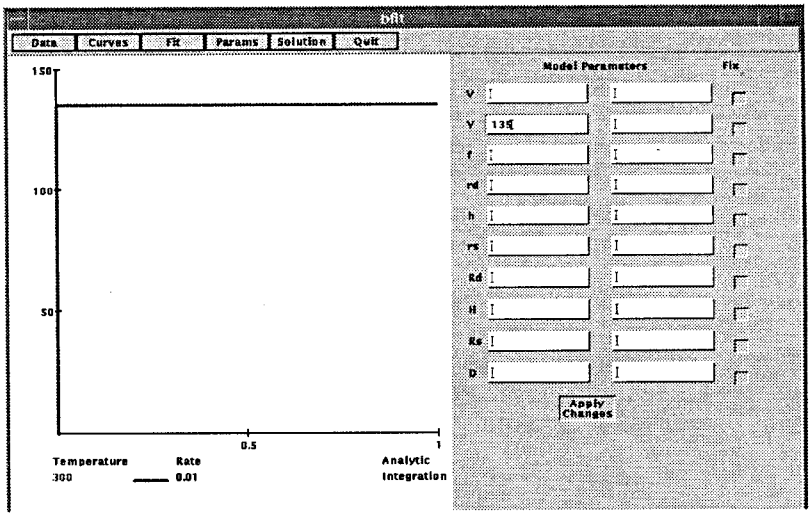


FIGURE 2. Elastic-perfectly plastic response

Plastic Hardening

You should now see a plot of stress versus strain. It's not too interesting yet, but we haven't done much either. Lets add a little isotropic hardening. Enter 150 under Model Parameters next to H and click on Apply Changes. Lets also limit the range of strain, so pick Curves from the menu bar and select Specify Scale. This brings up a window where you can enter the maximum strain to be plotted, enter .4 (for 40% strain) and click on OK. You will need to click on Apply Changes for all of this to take effect. In general, if you think something should change and it hasn't, click on this button to make the change take place.

We can add some kinematic hardening by entering 50 next to *h* under Model Parameters and click on Apply Changes. Change h to 0 and *H* to 200. Notice that the result is the same. In a uniaxial problem, kinematic and isotropic hardening behave the same. This is important to remember and can cause problems when we use the program to fit the model to data.

Rate Dependent Yield Strength

Now lets add some rate dependence to the yield strength. First lets ask for a plot of another strain rate, so under Curves, select Add Curve and enter temperature of 300 and a strain rate of 0.1, this will show two curves but they will be superimposed on each other.

The rate dependent part of yield stress is of the form $V\,\mathrm{asinh}(|D^p|/f)$ so lets add a value of 1.e-5 for f and 10 for *V*. Since that increases the yield strength by about 75 for a strain rate of .01, lets also change *Y* to 60. To see the result, click on Apply Changes.

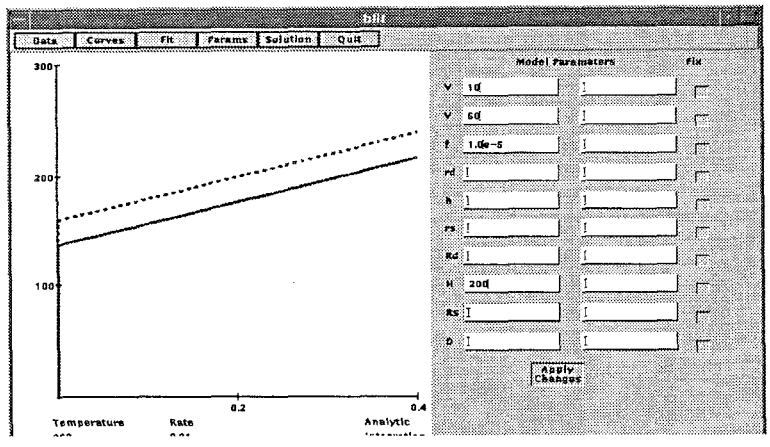


FIGURE 3. Constant hardening with rate dependent yield strength

Recovery

Set *h* to 0, and *H* to 200, and change the maximum strain to 1 (use Specify Scale under Curves). To see the effect of recovery, enter .04 next to *Rd*, and click Apply. This shows identical recovery for each curve. Now reset *Rd* to 0 and enter .004 next to *Rs* and click on Apply to see the effect of the rate dependent recovery term.

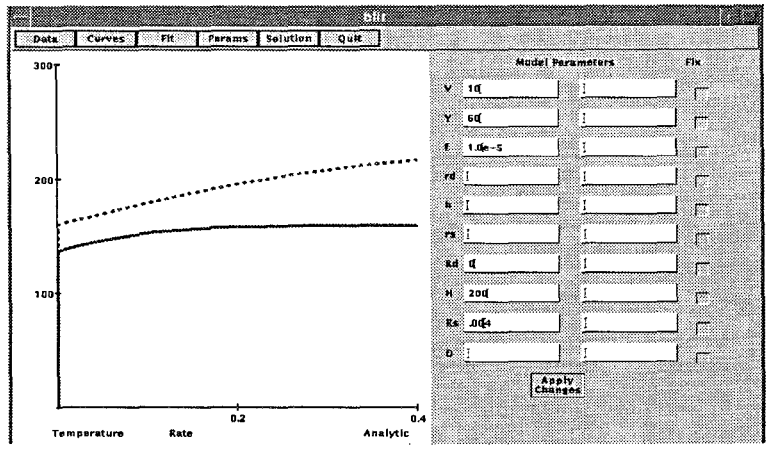


FIGURE 4. Rate dependent recovery

Isotropic hardening and recovery are determined by an equation of the form $\dot{\kappa} = C(A^2 - \kappa^2)$ where the coefficients $C = R_s + R_d|\dot{\varepsilon}_p|$ and $A^2 = (H|\dot{\varepsilon}_p|)/C$. As long as kappa starts out less than A, kappa will increase to the steady state value of A. However, if we initialize kappa to a value greater than A, it will decrease to its steady state value. Normally kappa starts out at zero, however you can specify an initial value by choosing Params on the menu bar and selecting initialize kappa. We can make use of this to create an apparent softening. For the current values, A turns out to be 22 for the .01 rate and 70 for the .1 rate. Try initializing kappa to values of 20, 40, 60, and 80 and observe the results. The term C controls the rate at which recovery occurs, so to get a slower rate, we need to adjust the other parameters. Try setting *Rs* to .00005 and then initialize kappa to 400. Now if we add some short term hardening we can get a curve that initially hardens and then softens. Try setting *h*=2000 and *rs*=.0006, and you should get the curves shown below. See if you can figure out how to get both curves to exhibit this "softening" behavior.

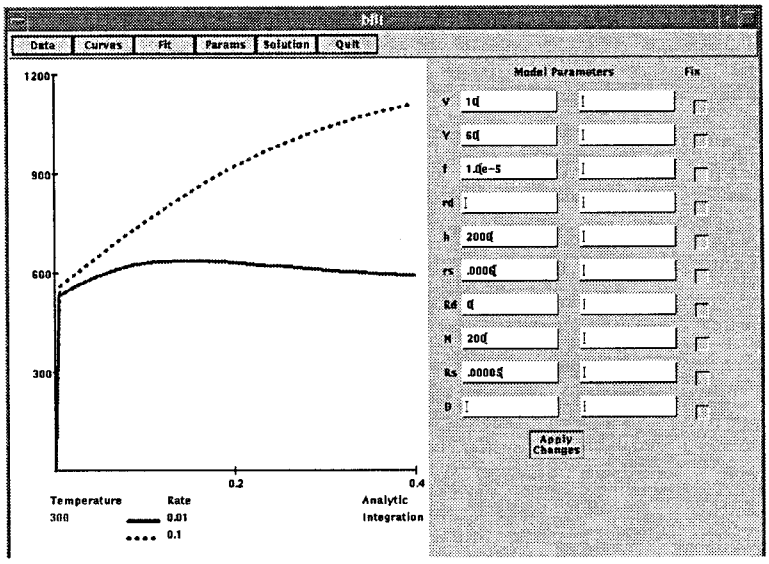


FIGURE 5. Hardening with softening at the lower rate

Fitting Data

A Sample Session

Lets go through a sample session of fitting data. If you are just starting a session, you will need to enter values of Young's modulus and Poisson's ratio. If you are continuing from the previous session, you can just start from there and you won't need to enter those values, although you should remove the old curves (under Curves).

To become familiar with the fitting part of the program we will use a fairly well behaved data set that should be in the same directory as the bfit program. Pick the Data button, and then select Read New Data under Uniaxial. A popup menu will appear to specify the form of the data file. The sample data file has stress, strain, strainrate and temperature on each record (line) so check the first format in the list (it should already be selected). There is also an option to preview the data, this provides some capability to limit the data. Since the data set we are using is fairly sparse, we won't use this (it is initially set as a default, so you must click on it and to deselect it). Now click on OK. The next popup gives you an opportunity to change units. The sample data is in MPa and we will be working in those units - so select MPa for both input and output (these should already be selected), and click the OK button. Next, a standard Motif file selector will appear.

Unless you are running from the directory containing the data you want to fit, you will need to traverse through directories to specify the file you want to use. There are several ways to specify a file: you can simply remove what is in the area below the word "selection" and type in the full path and file name in this region and then click on OK; or you can remove and type in the full path to the directory desired in the box below the word "filter" and then pick the filter button and finally scroll through the list of files in that directory and pick the one you want and then click on OK; or you can move through directories by scrolling the list of directories that are immediately accessible and select the one closest to where you want to be (dir/.. will move you up one level) and click on filter until you get to the desired directory and then you can scroll through and select the correct file. Whatever method you choose, you need to find the file many.dat which should be in the directory containing the bfit program.

You should now see a plot of the data (four sets of points). If they don't appear, click on Apply Changes.

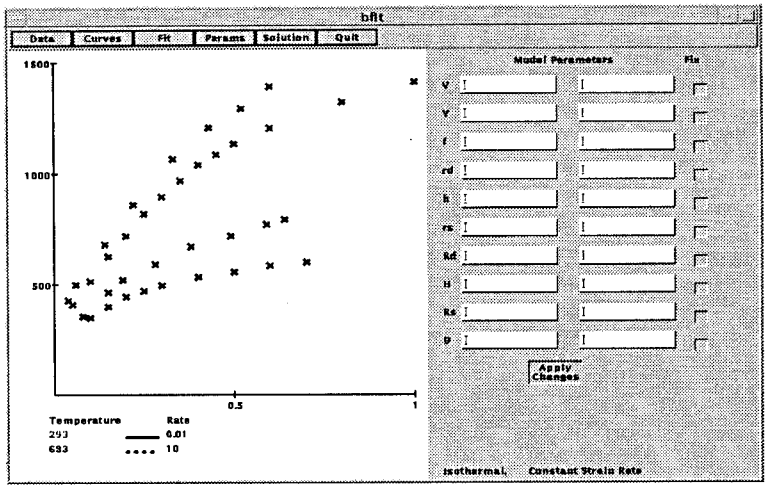


FIGURE 6. Data to be fit

The heart of the fitting section is a non-linear least-squares program developed at Sandia Laboratories [5]. Unlike linear least-squares procedures, a non-linear procedure needs a starting guess at the parameters to be fit, and unfortunately does not guarantee the absolutely "best" fit, but will only give a fit that is a "local" minimum, so the better your first guess, the better the fit will be.

The code has been designed to help you make a first guess at the parameters. You can just select Estimate model parameters from the Params menu and this will often give you a fairly good first guess. However if you have data for more than one temperature, it is better to fit two or more temperatures individually and then use those fits to estimate the temperature dependence of the fit. Fitting the extreme temperatures is usually the best approach.

To fit the data at just one temperature, select Restrict Data under the Data menu. A popup screen will appear listing the temperatures. Pick the 293 temperature and click on OK. You may have to click the Apply button for the reduced data set to be plotted. Now select Estimate model parameters form the Params menu and the code will estimate a set of parameters for you, display them on the screen, and plot the curves using those values. In this case it is not a very good fit but it is a place to start.

The least squares procedure can have trouble if you try to fit all of the parameters at once. I have found the best approach is to fix most of the parameters (the buttons to the far right) and just fit about three at a time. Since the yield stress looks fairly good, I would fix the first three and the last four parameters, and select Use Current Constraints under the Fit menu. The new fit is much better. You can monitor the improvement in fit by looking at the maximum and average residual displayed at the bottom. Now fix those parameters you just fit and unfix the first two parameters. This gives only a slight improvement, but now unfixing the *rd, h* and *rs* parameters as well and fitting gives a

very good fit. Some further improvements can be obtained by now fixing the first six parameters and fitting the last three parameters.

When you are satisfied with this fit, restore the full data set (pick Restore Data from the Data menu.) Restore data causes the program to remember the fit we got at the 293 temperature. Then, restrict the data to the 693 temperature and follow the same procedure to obtain a fit to this data beginning with estimate curves, and finally restore the data again.

At this point if you select Estimate model parameters from the Params menu, the code will use the two single temperature fits to get a temperature dependent fit and will display the values and the curves.

Notice, that the temperature dependent part of V is negative. This may not be acceptable (if you use this model for higher or lower temperatures than in the data you might see a temperature dependence of the yield stress that is wrong or at least not very believable). Try setting this value to zero (click Apply Changes to see the result), and then fit just the first two parameters. This should give a better fit.

Often if a parameter is set to zero, the least squares procedure won't change it, try setting the temperature term for V to one and fitting the parameters again (remember, you *must* click on Apply Changes for this change to be recognized by the code). This will probably result in a negative value again. To avoid this you can use the constraints. Set the value to one again (click Apply) and choose Add Constraints from the Fit menu. The temperature part of V is the second parameter, so you will want to constrain c2>0, so enter a zero to the left of c2 in the constraint window and click OK. Now if you select fit you will get the best fit it can obtain using a positive value of c2.

Again you can fix the first three and last three parameters and fit *rs*, *h* and *rd*. Then unfix the first three and fit it and so on until you get a fit you like. You can also try changing some of the values yourself and see what happens. Once you have a fit you are happy with, you can save it by selecting Hard Copy under the Curve menu. This will save a postscript image in the file bfit.ps. Using this option multiple times will concatenate plots. However, it will overwrite any bfit.ps files from previous runs. You can also save

the fit parameters on a readable (ASCII) file by selecting Save parameters under the parameters menu.

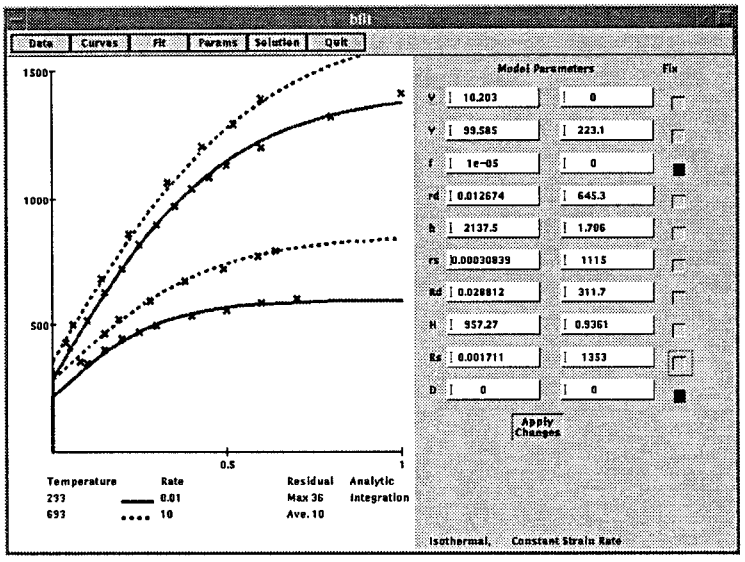


FIGURE 7. Finished fit

Temperature Dependence

Sometimes when fitting data you may have trouble getting the desired temperature dependence. This can be overcome, but it requires an understanding of the way temperature dependence is built into the model.

The Temperature dependence of each of the parameters is shown in table 1.

TABLE 1. Temperature dependence

V	$c_1 \exp(-c_2/T)$
Y	$c_3 \exp(c_4/T)([1 + (\tanh\langle c_{19}\langle c_{20} - T\rangle\rangle)]/2)$
f	$c_5 \exp(-c_6/T)$
rd	$c_7 \exp(-c_8/T)$
h	$c_9 - c_{10}T$
rs	$c_{11} \exp(-c_{12}/T)$
Rd	$c_{13} \exp(-c_{14}/T)$
H	$c_{15} - c_{16}T$
Rs	$c_{17} \exp(-c_{18}/T)$

The behavior of $\exp\left(-\frac{c}{T}\right)$ can be seen in fig. 8 while the behavior of $\exp\left(\frac{c}{T}\right)$ can be seen in fig. 9.

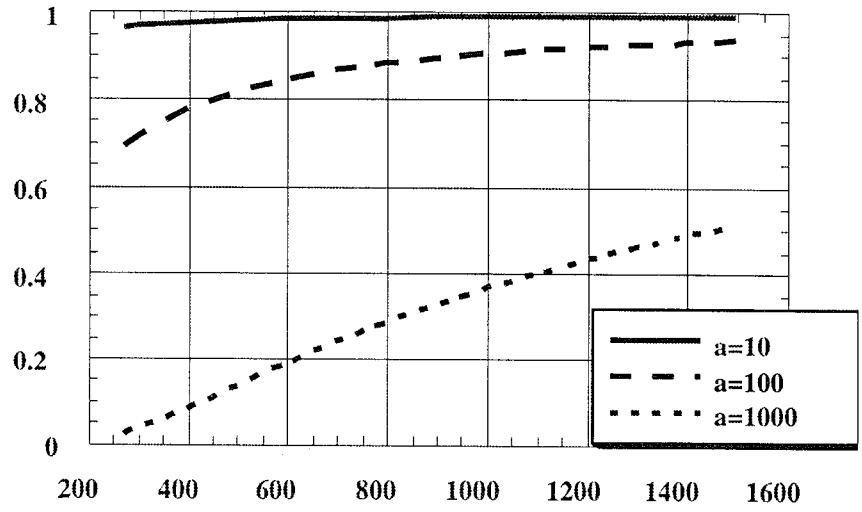


FIGURE 8. $\exp(-a/T)$

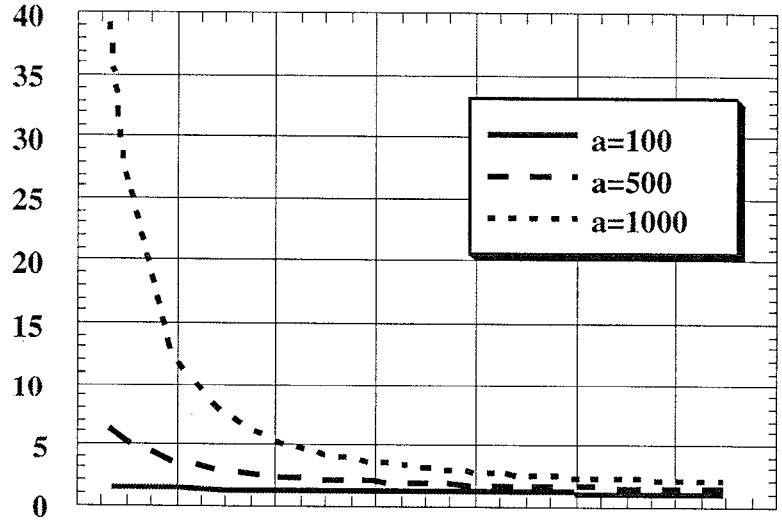


FIGURE 9. $\exp(a/T)$

As you can see, both exponential terms tend asymptotically to one. The negative form increases to one while the positive form decreases to one. Larger parameter values move the approach point further out on the temperature scale.

Over a large temperature range, the yield strength of a material is often not of this form, but instead will have a sort of backward s shape. For this reason an adjustment using a hyperbolic tangent of the form $1 + \tanh(c_{19}(c_{20} - T))$ where c_{20} is the temperature where the yield strength drops. This hyperbolic tangent term is shown in figure 10.

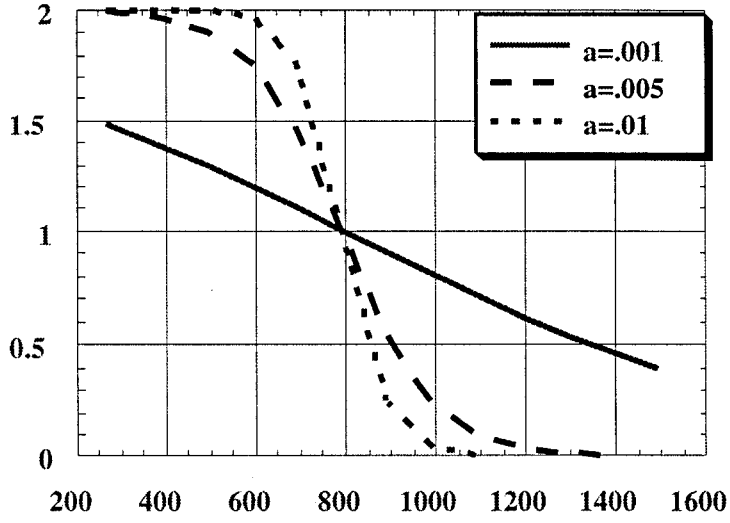


FIGURE 10. $1 + \tanh(a(800 - T))$

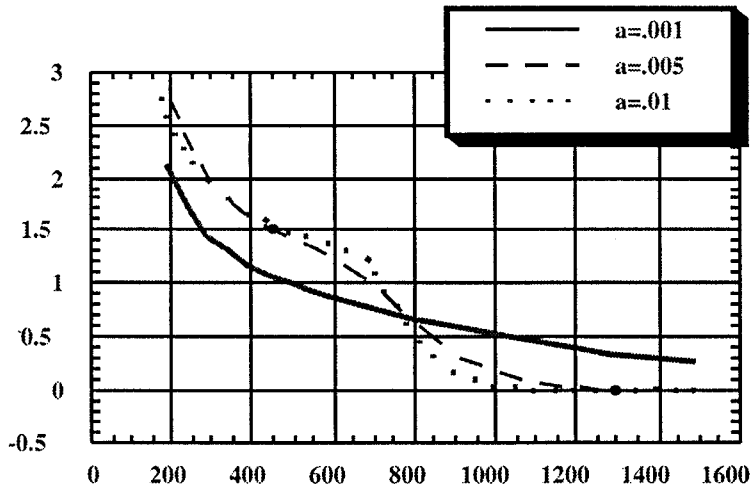


FIGURE 11. $\exp\left(\frac{200}{T}\right)\frac{(1 + \tanh(a(800 - T)))}{2}$

And finally you can see how this combines with the exponential function in figure 11.

If $c_{19} = 0$ this adjustment term is set to one. If you have fit three different temperatures the code will try to estimate values for c_{19} and c_{20}.These parameters are designated as D on the parameter display.

Code Options

Solution Options

Under the solution option, you can choose the type of loading and the method of solution. Of the integration options you can specify using the closed form integration or a numerical approximation only for uniaxial curves. The closed form solution is valid only for the isothermal constant strain rate problem. If you use the numerical integration you may specify the number of load steps and the error tolerance. More information on the integration is contained in the appendix.

Parameter Options

Moduli

Before the code can integrate the equations of motion it will need values of the Shear and Bulk moduli for the desired temperature. You may input a table of values that cover the temperature range of interest. As an alternative you may enter values for Young's modulus and Poisson's ratio, and the code will convert them for you. The program carries both sets and if you select either option it will display the current values. Thus, you could specify Shear and Bulk moduli at some temperatures and the click on the Young's modulus Poisson's ratio option and read off the equivalent values.

Inertial Effects

By default, the integration assumes a quasistatic problem (i.e. f/m=a=0). If you want to consider inertial effects you may provide the mass of a unit cube and the integration will solve $f = ma$ for uniaxial problems only.

Adiabatic Process

By default, the integration assumes the process to be isothermal. If you want to see the effect of heating due to plastic work you may enter a heat generation term. This term should be $(0.9/(\rho C_v))$. **Warning**: if you are using temperature dependent shear and bulk moduli be sure you have specified the shear and bulk moduli (or Young's modulus and Poisson's ratio) for a large enough temperature range to cover the temperatures being generated.

Parameter Estimation

If you have data displayed, the code can estimate material model parameters based on the initial slope of the data, the maximum stress and the differences in values for different strain rates (if they exist). For some data this is a fairly good guess, while in other cases the guess is abysmal and we're still working on this. Often when several temperatures are represented in the data it is advantageous to fit the data at several single temperatures (the restrict data option can be used). If more than one fit has been previously made at single temperatures, the code will estimate the parameters for the full range of temperatures by fitting the previously determined parameters with respect to temperature. This is often a fairly good fit.

Parameter Study

Once you have specified a set of parameters and the Bulk and Shear moduli, and have selected curves to display (or have data) you can request the parameter study option.

This will allow you to see the effect of changing a single parameter.You are given the choice of which parameter to vary, its minimum and maximum values and how many values to display.

Saved Parameters

You can save the parameters of a fit to an ASCII file (including the elastic moduli) by selecting Save Parameters. These values can be read back in using Get Parameters. This option also saves the elastic moduli that you used so even if you don't want to use the fit, it provides a way to avoid entering the elastic moduli each time you use the program.

Curve Options

Once you have specified the Shear and Bulk moduli and values for the model parameters, you can have the code calculate and display uniaxial stress strain curves. simple shear curves, single cycle load-unload curves, or creep curves.

For each type of curve you can either add a curve (to existing curves) or plot a new curve, removing any previous curves.

When adding curves to existing curves the code attempts to provide a key by color coding the temperatures and coding the strain rates by line type for up to 6 temperatures and 8 rates.

The scale option allows you to specify the maximum strain to be displayed for uniaxial or simple shear.

Hard Copy Plots

The hard copy option will provide a PostScript equivalent of the current plot on the file bfit.ps. Multiple requests will be concatenated together on that file. *Caution*: use of this option will overwrite any file created in a previous session if it still has that name.

Data Options

You can have the code read uniaxial data in one of two formats. Either the data file contains values of stress, strain, strain rate, temperature in that order with one set per record (line) or the file can contain just strain and stress with one set per record. Obviously if you specify the second form the program will ask you to specify the temperature and strain rate for that data file.

You can also obtain unit conversion by specifying input units of ksi or MPa and output or code units of ksi or MPa.

The options more data and new data allow you to add more data to data already read in or to start over with a new set of data. Warning: New means new - it will discard old data of any type.

If you have read in a lot of data it is sometimes useful to be able to look at the data corresponding to a single temperature. The restrict data option will present you with a list of temperatures and allow you to specify the desired one. It then displays only the curves corresponding to that temperature. Fitting will be done with this restricted data set also.

The restore data option will restore the full set of data to the condition it was in prior to using the restrict data option.

Data Preview

The program has a limited capability to modify the data. When data is read in, an option is to preview the data. When it is being preview, you have the option to limit the strain, which allows you to chop off any data beyond a given strain. The other option is to filter the data. This will produce a data set that describes the curve with fewer data points. If you choose this option you will be asked for an error value. The program tries to find points such that a line drawn between the points approximates the data between those points to a relative error not exceeding this error value. A choice of 0.01 seems to work quite well.

If you modify the data, you can save this modified data with the command Save Data. This saves the data in the stress, strain, rate, temperature format.

Fit Options

The program uses a non-linear least square routine to fit the data. This program requires a first guess at the parameters, and the better the guess, the better the least squares routine works. The routine works by incrementing each parameter slightly and approximating the matrix of partial derivatives of the errors of the fit with respect to the parameters. Using this information it tries to find a best direction to adjust all the parameters. It then uses a trial and error procedure to find how far in this direction to adjust the parameters. As you can see, this can take a lot of integrations and therefore take a lot of time. And it will only find a "local" minimum close to the starting guess.

You can help speed the fitting process by specifying the closed form solution (or a small number of integration steps if you insist on using numerical integration), and by not asking for all of the parameters to be fit at once.

Fixing Parameters

Since most of the parameters of the model are used in pairs, the parameters are presented in those pairs. To the right of each pair is a button. Activating this button will "fix" those parameters to their current value. You can often get good results by fitting just *rd* and *h*, and then *V* and *Y*, or adding *rs* to *rd* and *h*. If you fit a few parameters at a time until the fit looks good you can then usually perform a final fit allowing all or most of the parameters to change. Unfortunately this is not a procedure that can be automated, nor can rules be given that will work in all cases, you will just have to experiment with it.

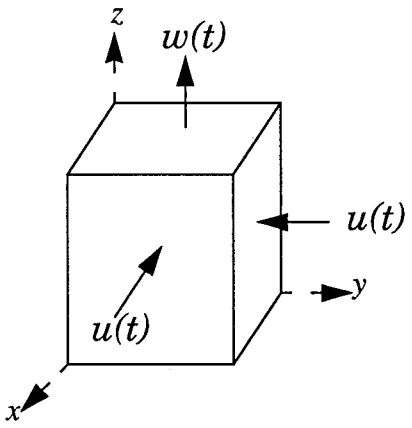
Constraints

If you wish, you can apply constraints to the parameters of the form $a < C_i < b$ where you specify the values of a and b. The fitting routine treats constraints with a penalty function and if it is having trouble with a fit, the penalty may not be big enough. Try adjusting the parameters to a fairly good fit by hand and then try to fit with constraints applied.

Calculations

Uniaxial Integration

Consider a single element, one unit cube with 3 adjoining surfaces fixed (i.e. an eighth of a cube two units on a side). If the top surface moves up with a displacement given by $w(t)$ the two free surfaces will move with a displacement $u(t)$



The true strain rate is given by

$$\dot{\varepsilon}_{xx} = \dot{\varepsilon}_{yy} = \frac{\dot{u}}{1+u}$$

$$\dot{\varepsilon}_{zz} = \frac{\dot{w}}{1+w}$$

For uniaxial tension (or compression) $w(t)$ is specified, so the integration problem is to determine $u(t)$ so that we satisfy either:

$\rho\ddot{u}(t) = \sigma_{xx}(1 + w(t))(1 + u(t))$ for the dynamic case, or

$\sigma_{xx} = 0$ for the quasistatic case.

Where the values of σ_{xx} and σ_{zz} are determined by the constitutive model.

The integration proceeds at each time step t advancing to time t+Δt by first estimating a new value $u(t + \Delta t) \approx u(t) + \dot{u}(t)\Delta t$. We then iterate on values of $u(t + \Delta t)$ until either $\sigma_{xx}(t + \Delta t) = 0$ in the quasistatic case, or until it satisfies the second order implicit formula

$$u(t + \Delta t) = u(t) + \dot{u}(t + \Delta t)\Delta t + \frac{\ddot{u}(t + \Delta t)\Delta t^2}{2}$$

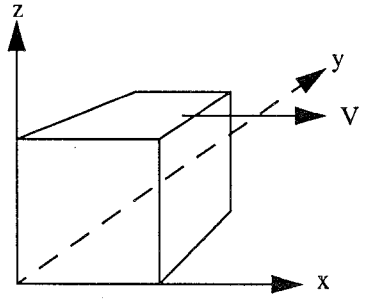
where

$$\dot{u}(t+\Delta t) = \frac{u(t+\Delta t) - u(t)}{\Delta t}$$

$$\ddot{u}(t+\Delta t) = \frac{\sigma_{xx}(t+\Delta t)[1+u(t+\Delta t)][1+w(t+\Delta t)]}{\rho}$$

Simple Shear Calculation

Consider a block, with motion at the top as shown.



The motion of a particle is given by

$$X(t) = X_0 + VtZ_0$$
$$Y(t) = Y_0$$
$$Z(t) = Z_0$$

The strain and strain rate tensors are then:

$$D = \begin{bmatrix} 0 & 0 & V(t/2) \\ 0 & 0 & 0 \\ V(t/2) & 0 & 0 \end{bmatrix} \qquad \dot{D} = \begin{bmatrix} 0 & 0 & V/2 \\ 0 & 0 & 0 \\ V/2 & 0 & 0 \end{bmatrix}$$

The rotation tensor is given by:

$$R = \begin{bmatrix} \cos(\gamma) & 0 & -\sin(\gamma) \\ 0 & 1 & 0 \\ \sin(\gamma) & 0 & \cos(\gamma) \end{bmatrix}$$

where $\sin(\gamma) = \dfrac{(tV)/2}{\sqrt{1+((tV)/2)^2}}$ and $\cos(\gamma) = \dfrac{1}{\sqrt{1+((tV)/2)^2}}$

The equation of state routine wants the unrotated tensor, so we calculate strain rate of R^TDR. It calculates σ which is then rotated back by $R\sigma R^T$. Bfit uses (and plots) effective stress and strain. these are calculated as

$$\bar{\sigma} = \frac{1}{\sqrt{2}}[(\sigma_1-\sigma_2)^2+(\sigma_2-\sigma_3)^2+(\sigma_3-\sigma_1)^2]+6(\sigma_4^2+\sigma_5^2+\sigma_6^2)]^{1/2}$$

$$\bar{\varepsilon} = \frac{\sqrt{2}}{3}[(\varepsilon_1-\varepsilon_2)^2+(\varepsilon_2-\varepsilon_3)^2+(\varepsilon_3-\varepsilon_1)^2+6(\varepsilon_4^2+\varepsilon_5^2+\varepsilon_6^2)]^{1/2}$$

In this case effective strain is then just $\bar{\varepsilon} = \sqrt{2}Vt$.

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